201-15773

NCIC OPPT/DC/USEPA/US
Sent by: JuanB Perez

01/10/2005 10:46 AM

To NCIC HPV@EPA
cc
bcc
Subject Re: HPV Submisssion

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US Environmental Protection Agency
Office of Pollution Prevention and Toxics Docket
Non-Confidential Information Center (MC 7407T)
(operated by ASRC Aerospace Corporation)
1301 Constitution Ave NW Room B146 EPA West
Washington DC 20460
phone 202-566-0280 * fax 202-566-0282 * e-mail oppt.ncic@epa.gov
EJ Rauckman <erauckman@charter.net>

EJ Rauckman
<erauckman@charter.net>
01/10/2005 10:44 AM

To NCIC OPPT@EPA, Rtk Chem@EPA
cc
Subject HPV Submisssion

HPV Coordinator,

On behalf of Solutia Inc Corporation, I am submitting the test plan and robust summaries for the HPV substances:

1,6-Hexanediaminium, N,N,N,N-tetrabutyl-N,N-diethyl-, bis(ethyl sulfate) (CAS Number 68052-49-3)

1,6-Hexanediaminium, N,N,N',N'-tetrabutyl-N, N'-diethyl-, dihydroxide (CAS Number 111960-92-0)

These are submitted as "paired chemicals" as they only vary by the type of salt of the quaternary amine.

These documents are in PDF format (unlocked). If you have any questions or require the documents in another format please contact me by email or telephone

Best regards,

Elmer Rauckman, PhD, DABT (for Solutia)

Toxicology and Regulatory Affairs

Freeburg IL 62243

rauckman@toxicsolutions.com

618-539-5380

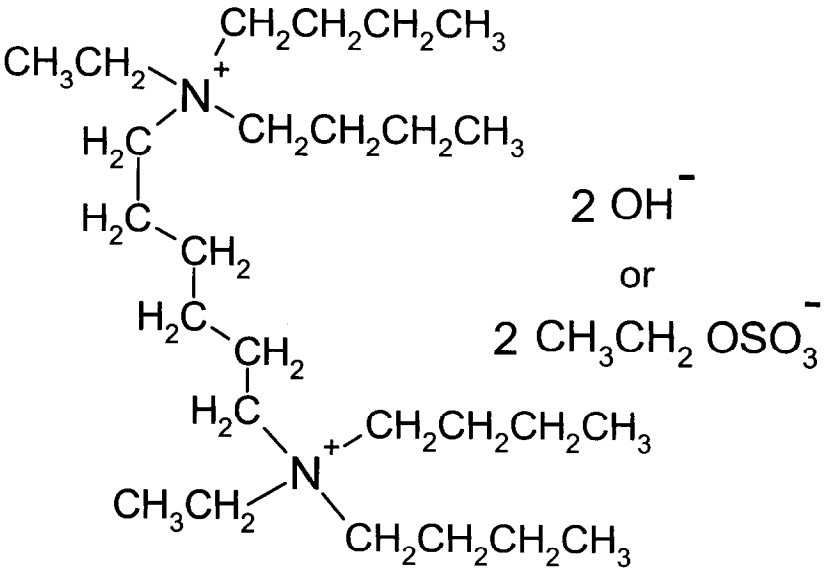

BQAOH and BQAES TP.pdf


BQAOH and BQAES RS.pdf

201-15773

1,6-Bis(dibutylethylammonium)hexane hydroxide
and
1,6-Bis(dibutylethylammonium)hexane ethylsulfate

CAS Number 111960-92-0 & 68052-49-3



U.S. EPA HPV Challenge Program Submission

Submitted by:

Solutia

Prepared by:
Toxicology and Regulatory Affairs
1201 Anise Court
Freeburg IL 62243
618-539-5280

30 December 2004

Table of Contents

Executive Overview

1,6-Bis(dibutylethylammonium)hexane hydroxide (BQAOH), CAS no. 111960-92-0 and 1,6-Bis(dibutylethylammonium)hexane ethylsulfate (BQAES), CAS no. 68052-49-3 are aliphatic quaternary amines that are produced by Solutia for internal use at only one site. All BQAES is converted to BQAOH that is used as a process aid in the manufacture of adiponitrile, which is a intermediate in Solutia's manufacturing process for nylon-6,6. Solutia produces BQAOH and BQAES at only one site and both are consumed at that site. Some of the BQAOH is disposed by processing in a wastewater treatment plant. This represents the only opportunity for the material to leave the manufacturing site; however, analytical determinations indicate that BQAOH is not discharged, nor processed in high enough concentration to interfere with the bacterial flora in the wastewater treatment plant. Worker exposure is minimized by the use of closed systems and mandated personal protective equipment.

These materials are known to be corrosive to skin and eyes and potentially lethal upon dermal exposure and, based on SAR, are assumed toxic to aquatic species in the environment and to the bacterial flora in a wastewater treatment plant at high levels. Because of these nefarious properties, a high standard of engineering controls, personal-protection requirements and wastewater treatment safeguards have been implemented to protect workers and the environment.

As produced and handled, both BQAOH and BQAES are aqueous solutions containing approximately 4 to 50% of quaternary amine salt. Both are colorless liquids with freezing points slightly below 0°C and boiling points slightly above 100°C. The quaternary amine salts themselves are solids with high melting points and very low vapor pressures. Both salts are water-soluble and the quaternary compounds have an estimated $K_{o/w}$ of 0.13, which indicates little potential for bioaccumulation in the environment. The solutions are clear liquids with a slight amine odor. BQAOH and BAQES both have very low volatility (estimated vapor pressure less than 0.00000001 hPa @ 25˚C) and are water-soluble.

If released into the environment, based on physicochemical properties, neither has significant potential to bioaccumulate (Log $K_{o/w}$ 0.13) and both will distribute primarily to water. Both materials are considered water stable but neither is expected to be resistant to biodegradation. Although volatilization to the atmosphere is not anticipated, the cations are expected to react rapidly with atmospheric hydroxyl radicals with a half-life of about 1.3 hours. Toxicity to aquatic species is predicted to be low using the ECOSAR model but testing is recommended to determine actual toxic potential.

The acute oral toxicity of BQAOH is moderate with an LD_{50} value of around 350 mg/kg found in a rat gavage study. BQAOH displayed a high degree of dermal toxicity in experimental animals giving a dermal LD_{50} in rabbits of only 22.5 mg/kg. Based on the high-level of acute toxicity and a presumed mechanism as a ganglionic blocker, repeated-dose, reproductive and developmental, and genotoxicity hazard assessments are derived using a "read-across" approach from similar compounds. These indicate little specific reproductive, developmental or genetic toxicity hazard. No studies have been conducted or proposed for BQAES as it is only a variation in the salt and, except for temporary storage, is not isolated.

It is concluded that the available information on the compounds and surrogates adequately fills all the data elements of the HPV Program for BQAOH and BQAES except for the biodegradation and aquatic toxicity endpoints. Studies to provide experimental data for these endpoints are recommended.

Testing Plan and Rationale

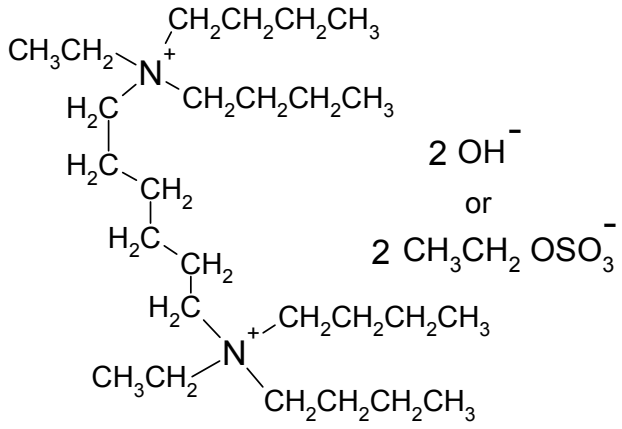
Testing Plan in Tabular Format

CAS No. 111960-92-0 BQAOH / HPV Endpoint	Information Available?	OECD Study ?	GLP Study?	Supporting Information?	Estimation Method?	Acceptable?	Testing Recommended?	
Physical Chemical								
Melting Point	Y	N	N	N	Y	Y	N	
Boiling Point	Y	N	N	N	Y	Y	N	
Vapor Pressure	Y	N	N	N	Y	Y	N	
Partition Coefficient	Y	N	N	N	Y	Y	N	
Water Solubility	Y	N	N	Y	N	Y	N	
Environmental & Fate								
Photo-Degradation	Y	N	N	N	Y	Y	N	
Water Stability	Y	N	N	Y	Y	Y	N	
Transport	Y	N	N	N	Y	Y	N	
Biodegradation	N	N	N	Y	N	N	Y	
Ecotoxicity								
Acute Fish	Y	N	N	N	Y	N	Y	
Acute Invertebrate	N	N	N	N	N	N	Y	
Acute Algae	N	N	N	N	N	N	Y	
Toxicity								
Acute	Y	N	N	Y	N	Y	N	
Repeated Dose	Y	N	Y	Y	Y	Y	N	
Genetic Toxicology *"in vitro"*	Y	N	Y	Y	Y	Y	N	
Genetic Toxicology "*in vivo*"	Y	N	Y	Y	Y	Y	N	
Reproductive	N	N	Y	Y	Y	Y	N	
Developmental	Y	N	Y	Y	Y	Y	N	

Introduction

1,6-Bis(dibutylethylammonium)hexane hydroxide (BQAOH), CAS no. 111960-92-0 and 1,6-Bis(dibutylethylammonium)hexane ethylsulfate (BQAES), CAS no. 68052-49-3 are aliphatic quaternary amines that are made and used by Solutia at one site. BQAES is an intermediate in the reaction sequence used to produce BQAOH. BQAOH is consumed on site as an aid in the electrochemical reaction used to produce adiponitrile, which is a intermediate in Solutia's manufacturing process for nylon-6,6.

The structures are shown below:



BQAOH and BQAES

BQAOH (CASNO 111960-92-0) is also known as (1):

- 1,6-Bis(dibutylethylammonium)hexane hydroxide
- 1,6-Bis(dibutylethylammonium)hexane dihydroxide
- 1,6-Hexanediaminium, N,N,N',N'-tetrabutyl-N,N'-diethyl-, dihydroxide (9CI)

BQAES (CASNO 68052-49-3) is also known as (2):

- 1,6-Bis(dibutylethylammonium)hexane ethylsulfate
- Tetrabutyldiethylhexamethylenediammonium ethylsulfate
- 1,6-Hexanediaminium, N,N,N',N'-tetrabutyl-N,N'-diethyl-, bis(ethylsulfate) (9CI)

All BQAES that is produced is converted to BQAOH that is used as a process aid in the manufacture of adiponitrile, which is a intermediate in Solutia's manufacturing process for nylon-6,6. Solutia produces BQAOH and BQAES at only one manufacturing site and both are fully consumed at that site. Some of the BQAOH is

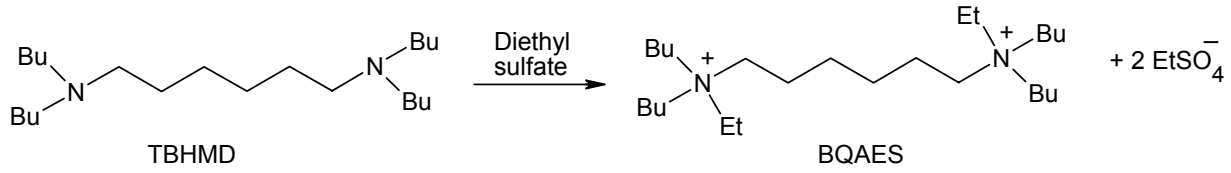
disposed by processing in a wastewater treatment plant. This represents the only opportunity for the material to leave the manufacturing site; however, analytical determinations indicate that BQAOH is not discharged, nor processed in high enough concentration to interfere with the bacterial flora in the wastewater treatment plant. Worker exposure is minimized by the use of closed systems and mandated personal protective equipment.

These materials are known to be corrosive to skin and eyes and potentially lethal upon dermal exposure and, based on SAR, are assumed toxic to aquatic species in the environment and to the bacterial flora in a wastewater treatment plant. Because of these nefarious properties, a high standard of engineering controls and personal-protection requirements have been implemented to protect workers and the environment. Exposure in industrial applications is limited by process controls, stringent protective equipment requirements and a very low vapor pressure. The number of workers possibly exposed to these chemicals is limited to about three per work shift.

No studies have been conducted or proposed for BQAES as it is only a variation in the salt and, except for temporary storage, is not isolated.

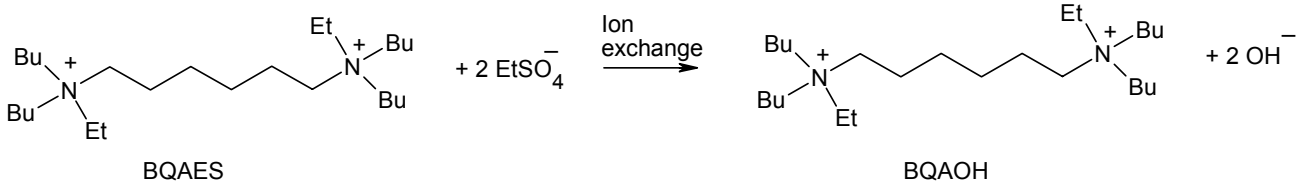
Chemistry of Manufacture

BQAES is produced by the reaction of N,N,N',N'-tetrabutylhexamethylene diamine (TBHMD) with ethyl sulfate as shown below.



TBHMD BQAES

BQAOH is made by an ion exchange reaction to convert the sulfate to the hydroxide.



BQAES BQAOH

All the BQAES produced is converted to BQAOH and all the BQAOH produced is used on site as a production aid in the manufacture of adiponitrile. Although there is some temporary storage of BQAES in a holding tank, it can be considered essentially a closed-system intermediate and BQAOH can be considered a site-limited intermediate. After its use as a production aid, about half the BQAOH is burned as part of an organic waste stream and about half goes with a wastewater stream to the on-site wastewater treatment plant

Physicochemical Data

Physicochemical data for BQAES and BQAOH are available from the manufacturer and from estimates.

Table 1: Physicochemical Properties of BQAES and BQAOH

Parameter	BQAES	BQAOH
Melting Point	ca. 300-350° C as solid (3) ca. -6° C as aqueous soln (4)	ca. 300-350° C as solid (3) ca. -3° C as aqueous soln (4)
Boiling Point (aqueous solution)	ca. 100-102°C @ 1027 hPa (5)	ca. 100-101°C @ 1027 hPa (5)
Vapor Pressure	negligible @ 25˚ C (6)	negligible @ 25˚ C (6)
Partition Coefficient Cation	Log $K_{o/w}$ = 0.13 (7)	Log $K_{o/w}$ = 0.13 (7)
Water Solubility	>10,000 mg/L @ 25° C (8)	>10,000 mg/L @ 25° C (9)

These properties indicate that at ambient temperatures both BQAES and BQAOH are non-volatile solids with high water solubility. The values of the partition coefficients, suggests that both will partition preferentially into water; therefore, on the basis of only the octanol-water partition coefficient, BQAES and BQAOH are considered to have minimal potential for bioaccumulation. As both materials are handled and used as aqueous solutions, the estimated boiling and melting point of the solutions were calculated from the solute concentration and given in Table 1. As organic salts, in the anhydrous form neither is expected to have a distinct boiling point as most organic salts decompose before boiling.

Regarding BQAES, which is an ethylsulfate salt, the values for the $K_{o/w}$, melting point and vapor pressure were independently calculated for the cation and anion. Only the values for the cation (quaternary amine) are shown in the table, while both values are given in the robust summaries.

Recommendation: No additional physicochemical studies are recommended. The available data fill the HPV required data elements.

Environmental Fate and Pathways

Photodegradation was estimated by examination of the structure for chromophores that would indicate direct photolysis and indirect photolysis was estimated using version 1.90 of the Atmospheric Oxidation Program for Microsoft Windows (AOPWIN) that estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The estimated rate constant is used to

calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radical. The program produced an estimated rate constant of 98.4 E-12 cm^3/molecule-sec for the quaternary amine, which is the same in BQAOH and BQAES. Using the default atmospheric hydroxyl radical concentration in APOWIN and the estimated rate constant for reaction of the quaternary amine portion of the molecule with hydroxyl radical, the estimated half-life of BQAOH vapor in air is approximately 1.3 hours (see accompanying robust summary for full details). In the case of BQAOH the anion is hydroxide, which will not further photolytically degrade. In the case of BQAES, the anion is ethylsulfate. The half-life of ethylsulfate (as the sodium salt) was estimated with the AOPWIN program as 13 days based on the default hydroxyl radical concentrations and an estimated rate constant of 0.82 E-12 cm^3/molecule-sec for reaction with atmospheric hydroxyl radical. It should be noted that since both materials have insignificant vapor pressures and high water solubilities, it is unlikely that release of vapor into the atmosphere will be significant for either material under plausible release scenarios.

Water stability has not been quantitatively determined for BQAOH or BQAES. Quantitative stability determinations (e.g. OECD 111) are considered unnecessary for compounds containing only non-hydrolysable groups. Under these conditions, the SIDS manual states that consideration should be given to using an estimation method. There is no evidence available in the literature that BQAOH or BQAES are unstable in water and they are in fact handled, stored and used as aqueous solutions. Regarding the quaternary amine cation, no specific data were found for water stability of similar quaternary amines. Assuming the reaction products of hydrolysis is the tertiary amine and either butanol or ethanol, the enthalpy of the reaction can be calculated using standard bond energies. As the number of reactants (2) is the same as the number of products (2), it can be assumed that entropy changes will be a minor consideration in the free energy change resulting from the hydrolysis reaction and the feasibility and rate of reaction can be estimated from enthalpy estimates. Conducting this calculation using standard bond energies and the hydrolysis reaction was estimated to be endothermic by more than 400 kJ/mole (see robust summary). With this scale of energy requirement, it can be assumed that the quaternary amine moiety will by hydrolytically stable under environmental conditions (that is it may be considered non-hydrolysable).

Regarding the anions, the BQAOH anion is the hydroxyl ion, which is considered fully hydrolyzed. The BQAES anion is monoethylsulfate and since it is known that diethyl sulfate hydrolyzes to ethanol and sulfate with a half-life of 1.7 hours (10), and because monoethylsulfate is an intermediate in this reaction, the hydrolysis half-life of this anion can safely be estimated as less than 1 day under environmental conditions (see robust summary for details).

Except for data showing ready biodegradation of diethyl sulfate in the MITI test (11), no definitive biodegradation data has been located for BQAOH or BQAES. Biodegradation studies of quaternary amines are limited as many of these materials are biocidal surfactants and are difficult to study using standard protocols. In the extensive book "Surfactant Biodegradation", Swisher (12) only devotes a short section to a discussion of the biodegradation of alkyl quaternary amines. This review, directed toward monoamino quaternary amines, notes that difficulties have been encountered due to bacterial toxicity. Biodegradation results for the alkyl quaternary amines are mixed but indications are that most of the ones tested are "ultimately biodegradable". As BQAOH and BQAES are

comprised primarily of linear alkyl groups and are not anticipated, based on their structures, to have significant surfactant or biocidal properties, they are anticipated to be biodegradable and this is confirmed by analytical investigations of wastewater at the plant. Definitive determination of the relative rate of biodegradation, however, will require testing; hence, biodegradation testing of BQAOH is recommended. As the quaternary amine structure of BQAOH and BQAES are identical and as diethylsulfate is known to be biodegradable, testing of only BQAOH is considered sufficient.

Theoretical Distribution (Fugacity) of BQAOH and BQAES in the environment was estimated using the MacKay EQC level III model found in EPIWIN set to estimate distribution after 100% release to water, which is the most likely scenario. The EPIWIN model was allowed to estimate physicochemical and fate parameters used in the calculations; however, these were verified for appropriateness before the final calculation was accepted. Because BQAES is a salt and is expected to dissociate in the environment, the cationic and anionic portions of the salt were independently modeled. (see robust summaries).

The results for both the cation and anion are similar, except for about 0.2% distributing to sediment, all the material remains in the water column. (13). A summary of these results is shown below in Table 2:

Environmental Compartment	**Species Modeled**	
	BQAOH and BQAES Cation	Sodium ethylsulfate
○ Air	< 0.01%	< 0.01%
○ Water	99.8%	99.8%
○ Soil	< 0.01%	< 0.01%
○ Sediment	0.2%	0.2%

Table 2. Distribution Estimates from EQC Level III Model

Recommendation: Considering the uncertainty in the ease of biodegradation for the BQAOH quaternary amine cation, an OECD 301 or 302 series study is recommended. No additional fate studies are recommended. The available data fill all other HPV required elements.

Ecotoxicity

No definitive data on the ecotoxicity of BQAOH or BQAES could be found. Although the EPA ECOSAR program estimated the LC_{50} for fish at 23,000 mg/L using the cationic surfactants model, the similarity of the

structure to cholinergic blocking agents suggests that there is a potential for acute toxicity to fish should the material be bioavailable. Regarding the ethylsulfate anion, since it is readily biodegradable and hydrolysable and will rapidly hydrolyze under environmental conditions to sulfate and ethanol, it may be considered well characterized. It is recommended that OECD-guideline fish, invertebrate and algal toxicity assays be conducted using BQAOH. Studies should use neutralized conditions to best represent actual environmental conditions. As the material is considered to be stable and highly soluble in water the use of nominal concentrations and static conditions is recommended for this screening-level hazard assessments.

Recommendation: Acute fish, invertebrate, and algal toxicity studies of BQAOH are recommended to provide information adequate for the purpose of the HPV program.

Health Effects

Acute Toxicity

Oral Exposure

The oral LD_{50} of BQAOH was determined to be approximately 350 mg/kg in Sprague-Dawley rats dosed by gavage with a 28% solution of BQAOH. Clinical signs in decedents were reported as rapidly increasing weakness, collapse and death occurring between 30 minutes and 120 minutes of administration. No clear cause of death could be identified at necropsy; the principle necropsy finding was hemorrhagic lung and liver. (14)

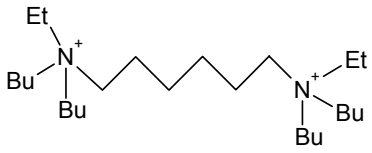
Dermal Exposure

The dermal LD_{50} of BQAOH was determined to be approximately 22.5 mg/kg in New Zealand white rabbits dosed with a 28% solution of BQAOH. Clinical signs in decedents were reported as rapidly increasing weakness, collapse and death occurring about 2 hours after administration. No clear cause of death could be identified at necropsy; the principle necropsy finding was hemorrhagic lungs. Furthermore, all six rabbits died after application of 0.5 ml of 28% aqueous solution in a skin-irritation study in which the solution was determined to be corrosive to skin. (14)

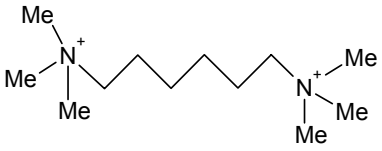
Relative to acute toxicity, the greater sensitivity of test animals by dermal exposure than by oral exposure is noted. This can be explained several ways including species difference, limited oral absorption or first-pass metabolism of the test material by the liver of rats. The most probably explanation is thought to be limited oral absorption as it is established that the absorption of quaternary compounds from the enteric tract is “incomplete and unpredictable” (15). Hexamethonium bromide, which has a similar structure and was FDA approved for treatment of hypertension between 1951 and 1972, shows a similar toxicity profile for oral versus subcutaneous treatment of rats. Its oral LD_{50} is 2891 mg/kg while the subcutaneous LD_{50} is only 200 mg/kg (RTECS). Another quaternary compound that is fatal at low dermal doses is tetramethylammonium hydroxide, which has an oral LD_{50} of 34-50 mg/kg in rats (16) and is fatal to rabbits when applied as a 2.75% solution (17) (estimated dermal LD_{50} <20 mg/kg). This demonstrates that charged quaternary ammonium compounds can be absorbed through the skin and cause mortality at very low doseage levels.

The similarity of the structure of BQAOH to the prototypical ganglionic blocking drug hexamethonium is obvious by examination of the structures below. The muscle paralyzing activities of quaternary amines were first described by Marshall in 1913 who described the “nicotine paralyzing” activity of tetraethylamine on ganglia (18). More than 30 years passed before the bis-quaternary ammonium salts were independently studied and developed by Barlow and Ing and reported in a 1948 publication (19) and by Paton and Zaimis in a 1952 publication (20). Hexamethonium was the “prototypical” agent described and was reported to have potent ganglionic blocking activity but minimal neuromuscular or muscarinic activity. In the subsequent years, many specific ganglionic and neuromuscular blocking agents have been developed and used, especially as an adjunct to anesthetic agents in surgery. Hill reviewed many of the active compounds and discussed structure –activity relationships (21); subsequently, a review in 2001 by Lee (22) extended the review and discussed conformational

contributions to specific activity. These reviews discuss several structural features that affect the nicotinic activity of amines. Relative to this discussion, important observations are that a very wide variety of structures have activity at the nicotinic receptor. The specific mode of activity can be depolarizing or non-depolarizing with bulkier compounds tending to be non-depolarizing. The amines do not have to be quaternary to have activity; potency generally follows the order: bis quaternary amines > bis amine with one nitrogen tertiary and one quaternary> bis tertiary amines> quaternary mono-amines. Depending on the structure, other cholinergic receptors can be affected most notably those of the cardiovascular system. An important determinant of the activity type (ganglionic or neuromuscular junction) and potency is the distance between the two charged nitrogen atoms. As both BQAOH and hexamethonium share a hexamethylene bridge between the quaternary nitrogens, they are anticipated to have similar pharmacological specificity. It is logical to speculate that BQAOH will show clear ganglionic blocking activity and is anticipated to cause mortality by blocking respiration at sufficiently high dose levels. This hypothesis is supported by the data showing rapid mortality in rats after oral administration and in rabbits after dermal administration with a lack of delayed deaths in both species. The low LD_{50} of BQAOH in rabbits also supports a specific pharmacological activity after dermal administration. It can therefore be concluded that the toxicity of BQAOH is most probably mediated by its activity as a ganglionic blocking agent.



BQAOH



Hexamethonium

Recommendation: No additional acute toxicity studies are recommended. The available data fill the HPV required endpoints for acute toxicity. Although the available studies do not meet all requirements of current OECD guidelines in all cases, the weight of evidence shows that the oral toxicity is significant and that the dermal toxicity is remarkably high.

Repeat Dose Toxicity

Repeated-dose studies have not been conducted on BQAOH or BQAES. Although chemicals produced at this volume within Solutia generally have a more complete data set, there are sound reasons why repeated-dose have not been conducted with these materials:

- These materials are highly toxic after acute exposure producing lethality and severe burns.
- These materials already carry the strongest possible label warnings.
- A high level of personal protective equipment is required when handling the materials.
- These materials are produced and consumed entirely on site.
- Findings of repeated-dose studies would not change handling procedures.
- Conduct of additional studies would unnecessarily expose laboratory workers to these acutely toxic materials.

For these reasons, and because additional mammalian testing would result in pain (the material is corrosive) and death of laboratory animals, additional mammalian testing cannot be recommended. For the purposes of the HPV program it recommended that surrogate compounds that already have data be used for filling the endpoints.

Quaternary ammonium compounds (QACs) are a recognized group of industrial chemicals used for their activity as surfactants and bactericides. EPA suggested in 1988 that the QACs could be divided into four groups and that toxicity studies would be facilitated by selecting a representative compound from each group for testing (23)

- Group I: Straight-chain alkyl or hydroxyalkyl QACs
- Group II: Alkyl dimethyl benzyl ammonium compounds
- Group III: Alkyl [di- and tri- chlorobenzyl] dimethyl ammonium compounds
- Group IV: Heterocyclic ammonium compounds

BQAOH and BQAES fall in Group I, although data from Group II QACs may still be applicable. Several observations lend support to using Group I and II QACs as surrogates for BQAOH and BQAES (24).

- Some produce remarkably higher toxicity by sq or ip routes than by oral administration
- Some show curare-like activity resulting in muscle paralysis causing rapid death without CNS effects
- Among the alkyl dimethyl benzyl ammonium compounds, shorter (e.g. C8) alkyl carbon chain compounds were more toxic than those with longer carbon chains and increase in carbon chain length beyond C16 markedly reduced toxicity.
- The rat oral LD_{50}'s for most QAC's are in the range of 250-1000 mg/kg
- Most QACs are strong skin and eye irritants in aqueous solutions.

This spectrum of activity is consistent with the acute toxicity data from BQAOH, suggesting commonality of mechanism for BQAOH with the Group I and Group II QAC's. Based on this, it is proposed that data from other QACs can be reasonably used to access the potential health effects of BQAOH and BQAES.

Didecyldimethylammonium chloride, CASNO 7173-51-5 (DDDMAC) has been designated by EPA as the representative chemical for toxicology studies for all dialkyl quaternaries. As BQAOH and BQAES have multiple alkyl groups associated with the quaternary nitrogen (two butyl and one ethyl) and as the empirical formulas for the cationic portion of BQAOH and BQAES ($C_{26}H_{58}N_2$) is similar to DDDMAC ($C_{22}H_{48}N$), DDDMAC was also selected as the principle surrogate for BQAOH and BQAES. Several other surrogates, however, are available and provide confirmatory evidence for the health effects assessment (25).

Oral Exposure

Didecyldimethylammonium chloride, CASNO 7173-51-5, DDDMAC was incorporated in the diet and fed to groups of 60 Sprague-Dawley rats of each sex for 104 weeks at 0, 300, 750, or 1500 ppm. Decreased bodyweight gain and food consumption was observed in each sex at 1500 ppm. Increased incidence in mesenteric lymph node pathology (blood in sinuses, hemosiderosis and histiocytosis) occurred in both sexes at 1500 ppm. Bile duct hyperplasia occurred in females at 1500 ppm. Treatment-related oncogenicity was not observed. The chronic NOEL was determined to be 750 ppm for rats of each sex (26).

Recommendation: No additional repeated-dose studies are recommended. The available data fill the HPV required endpoint for repeated-dose toxicity.

Genetic Toxicity

The SIDS/HPV requirement for genetic toxicity screening is for two end-points: generally one test sensitive for point mutation and one sensitive for chromosomal aberrations. In the case of these materials, adequate tests using various surrogate compounds have been conducted that cover both of these endpoints. As in the case of the repeated-dose assessment, the lack of potential exposure, the warning label and level of protective equipment utilized, the commonality of the quaternary amine groups in normal biochemical processes and the availability of consistently negative data on a variety of analogous compound indicate there is no need to conduct genotoxicity studies on BAQOH or BAQES. DDDMAC studies are proposed as a surrogate for filling the HPV genotoxicity data elements.

Genetic Toxicology in vitro

DDDMAC was tested in a CHO/HGPRT forward mutation assay at concentrations of 0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0 or 10.0 µg/ml without metabolic activation trial and at concentrations of 0, 1.0, 5.0, 10.0, 13.0, 15.0, 18.0, 20.0, 22.0 or 25.0 µg/ml with metabolic activation. Cell survivals were in an acceptable range. Neither assay showed an increase in mutant frequency (27).

DDDMAC was tested in an in vitro cytogenetic assay in the presence of activation (+S9) with Chinese Hamster ovary cells in duplicate at concentrations of 0, 2, 4, 8, or 16 µg/ml. In the absence of activation (no S9), concentrations for the first replicate were 0, 0.25, 0.5, 1.0, and 2.0 µg/ml and because these levels did not produce the expected toxicity and levels for the second replicate were increased to 0, 1.0, 2.0, 4.0, or 8.0 µg/ml. No adverse effects were reported either with or without S9 (28).

Genetic Toxicology in vivo

Metaphase chromosomes obtained from the bone marrow of CD rats treated with DDDMAC by gavage at doses of 0 or 600 mg/kg were analyzed for adverse effects at sampling times of 6, 24, and 48 hours. The positive control cyclophosphamide was administered at 40 mg/kg and bone marrow was sampled at 24 hours post treatment. No treatment-related effects to metaphase chromosomes were observed and positive controls gave the expected result (29).

A large number of genotoxicity studies, have been reported on other related QACs indicting a general lack of genotoxicity (30)

Recommendation: The SIDS requirement for genetic testing has been met as assays sensitive to both point mutation and to clastogenic effects have been conducted on related materials using acceptable protocols. No additional genotoxicity testing is recommended.

Reproductive Toxicity

As described under *Repeated Dose*, a surrogate chemical is recommended to fill this HPV endpoint.

A two-generation reproductive of DDDMAC was conducted by dosed feed using Sprague-Dawley (CD) rats (28/sex/dose) treated through two generations with 2 litters per generation at dose levels of 0, 300, 750, or 1500 ppm. Treatment began 10 weeks prior to mating. At 1500 ppm, reduced bodyweight gains and food consumption were observed for parental animals and pups displayed reduced bodyweight gain. The parental and maternal NOAL was 750 ppm.

Recommendation: No additional reproductive testing is recommended. The available data are sufficient to assess the reproductive toxicity of this material.

Developmental Toxicity

As described under *Repeated Dose*, a surrogate chemical is recommended to fill this HPV endpoint.

DDDMAC was tested for developmental toxicity in a rabbit study using 16 animals per group and doses of 0, 1.0, 3.0 or 10.0 mg/kg-day administered by gavage on days 6 - 18 of gestation. In this study, the maternal NOEL was determined to be 1.0 mg/kg. There were 4 deaths accompanied by labored respiration, gasping, sloughing of esophageal lining and stomach, and decreased weight gain at 10.0 mg/kg. At 3.0 mg/kg, audible respiration, hypoactivity and decreased weight gain was observed in the dams. The developmental NOEL was 3.0 mg/kg. At 10 mg/kg-day, there was an increased number of dead fetuses/litter and decreased fetal body weight.

Other QACs with similar structures have been tested for developmental toxicity and reported in the "Fatty Nitrogen Derived Cationics Category " and none have given positive results (30). In addition, developmental toxicity of the neuromuscular drugs has been reviewed by Schardein and found to be largely devoid of developmental toxicity (31).

Recommendation: No additional developmental toxicity testing is required as the available data are sufficient to assess the developmental toxicity of this material.

Conclusions

With regard to the parameters specified in the EPA HPV Challenge program, it is concluded that the available information fills all of the requirements for physicochemical parameters, and acute toxicity. As the materials have a high degree of acute toxicity after dermal administration (dermal rabbit LD_{50} of 22 mg/kg), and likely act at peripheral cholinergic sites to cause muscle paralysis, and are site-limited intermediates, additional health effect studies are not recommended. Additional studies would not impact the warning label, handling recommendation, or requirements for personal protective equipment that are already in place for these acutely toxic materials. It is proposed that rather then expose testing laboratory personnel to the known hazards of BQAOH and BAQES, the HPV data elements for repeated dose toxicity, reproductive and developmental toxicity and genotoxicity be filled using data from surrogate quaternary amines. It is recommended, however, that the HPV data elements of biodegradation and aquatic toxicity be filled by appropriate OECD-guideline testing on BQAOH.

References

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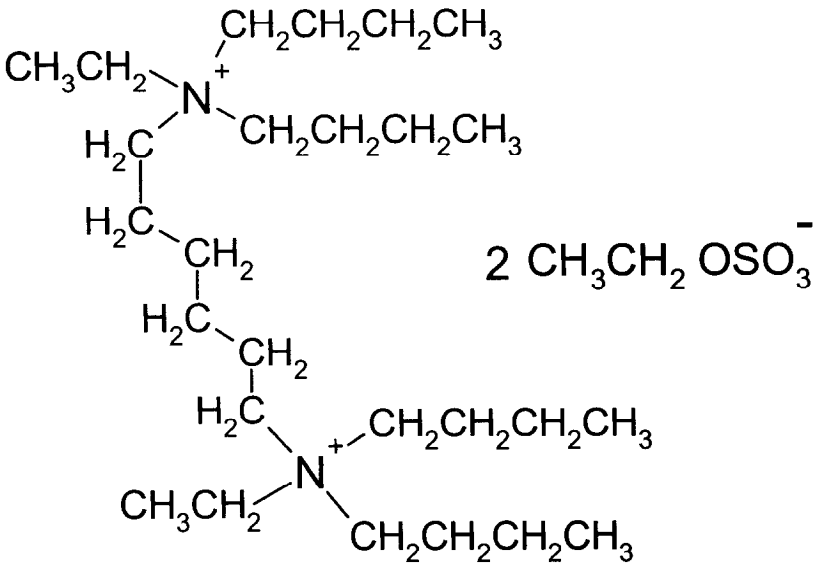
HPV Data Set



BQAES

Existing Chemical	:	ID: 68052-49-3
CAS No.	:	68052-49-3
EINECS Name	:	S,S'-diethyl N,N'-hexane-1,6-diylbis(dibutylethylammonium) disulphate
EC No.	:	268-327-3
Molecular Formula	:	C26H58N2.2C2H5O4S

Producer related part

Company	:	Solutia Inc
Creation date	:	02.01.2005

Substance related part

Company	:	Toxicology and Regulatory Affairs
Creation date	:	02.01.2005
Status	:	Prepared by: Toxicology and Regulatory Affairs Freeburg IL 62243 rauckman@toxicsolutions.com
Memo	:	BQAES
Printing date	:	09.01.2005
Revision date	:	
Date of last update	:	04.01.2005
Number of pages	:	17

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	manufacturer
Name	:	Soluita Inc
Contact person	:	
Date	:	
Street	:	
Town	:	
Country	:	
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

04.01.2005

1.2 SYNONYMS AND TRADENAMES

2.1 MELTING POINT

Value : <= 318 °C
Sublimation :
Method : other: Calculated
Year :
GLP :
Test substance : other TS

Method :

This material is produced, handled and disposed of as an aqueous solution containing up to 48% organic content. The melting point for the solid material has not been recorded as it is not isolated, but as an impure salt it is expected to be relatively high and variable. For the purpose of an HPV program, the melting point of the solid was estimated with the MPBPWIN (v 1.4) program. This estimate is considered an upper limit of the practical melting point for the solid. Due to limitations of the estimation software the cation and anion (as the sodium salt) portions of the molecule was separately estimated.

Result :

MPBPWIN (v1.40) Program Results:
==========
CATION
Experimental Database Structure Match: no data

SMILES : CCCCN(CCCC)(CC)CCCCCCN(CCCC)(CCCC)(CC)
CHEM : BQAOH++ (twice charged form)
MOL FOR: C26 H58 N2
MOL WT : 398.77

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	6	-CH3	-5.10	-30.60
Group	20	-CH2-	11.27	225.40
Group	2	>N< (+5)	340.00	680.00
*		Equation Constant		122.50
RESULT		MELTING POINT in deg Kelvin		997.30
RESULT-limit		MELTING POINT in deg Kelvin		623.00
		MELTING POINT in deg C		349.84

Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 309.98 deg C (Gold and Ogle Method)
Mean Melt Pt : 329.91 deg C (Joback; Gold,Ogle Methods)
Selected MP: 317.95 deg C (Weighted Value)

ANION

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	1	-CH3	-5.10	-5.10
Group	1	-CH2-	11.27	11.27
Group	2	-O- (nonring)	22.23	44.46
Group	1	>S(=O)(=O)	150.00	150.00
Group	1	Metal (Na,K,Li)	350.00	350.00
*		Equation Constant		122.50
RESULT		MELTING POINT in deg Kelvin		673.13
RESULT-limit		MELTING POINT in deg Kelvin		623.00
		MELTING POINT in deg C		349.84

Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 162.22 deg C (Gold and Ogle Method)
Mean Melt Pt : 256.03 deg C (Joback; Gold,Ogle Methods)
Selected MP: 199.75 deg C (Weighted Value)

Test substance :

Solid portion of aqueous solution, BQAES CASNO 688052-49-3

Conclusion :

The actual melting point of the solid portion of this material is expected to vary, depending on the impurity level, with a maximum of 318 °C

Reliability : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag : Critical study for SIDS endpoint
02.01.2005 (4)

Value : ca. -6.4 °C
Sublimation :
Method : other: Calculated for solution
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4

Method :

The material as produced is an aqueous solution containing up to 48% BQAOH. The practical freezing point of the solution is a function of the solvent's freezing point and the freezing point depression caused by the solute. An approximate freezing point can be calculated based on the molal freezing-point depression constant for water of 1.86°C

Result :

For a 48% solution of BQAES in water the approximate molality is 1.1. Considering that there could be up to three ions, the freezing point depression could be as great as 6.4°C.

Conclusion :

The freezing point range for this material as an aqueous solution is 0 to -6.4°C; however, limits on the solubility could cause precipitated solid formation prior to freezing.

Reliability : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag : Critical study for SIDS endpoint
02.01.2005 (1)

2.2 BOILING POINT

Value : ca. 100 - 102 °C at
Decomposition :
Method : other: Calculated for solution
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4

Method :
The material as produced is an aqueous solution containing up to 48% BQAES. The practical boiling point of the solution is a function of the solvent's boiling point and the boiling point elevation caused by the solute. An approximate boiling point can be calculated based on the molal boiling-point elevation constant for water of 0.52°C/m.

Remark :
The solid material is expected to decompose before boiling as it is a high molecular weight salt.

Result :
For a 48% solution of BQAOH in water, the approximate molality is 01.11. Considering that there could be up to three ions, the boiling-point elevation could be as great as 1.8°C.

Conclusion :
The initial boiling point range for this material as an aqueous solution is 100 to 102°C.

Reliability : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag : Critical study for SIDS endpoint
02.01.2005 (1)

2.3 DENSITY

2.4 VAPOUR PRESSURE

Value : < .00000001 hPa at 25 °C
Decomposition :
Method : other (calculated)
Year :
GLP :
Test substance : other TS

:

Method The vapor pressure for a charged salt is expected to be negligible. In addition, as this material is produced and handled as an aqueous solution, the Henry's law constant is a more important factor for exposure consideration from bulk material or material that is introduced into the water column. EPIWIN was used to provide estimates for both the vapor pressure and the Henry's law constant. Due to limitations of the estimation software the cation and anion (as the sodium salt) portions of the molecule was separately estimated.

Result :

```
CATION

MPBPWIN (v1.40) Program Results:
==============================
Experimental Database Structure Match:  no data

SMILES : CCCCN(CCCC)(CC)CCCCCCN(CCCC)(CCCC)(CC)
CHEM   : BQAOH++  (twice charged form)
MOL FOR: C26 H58 N2
MOL WT : 398.77
----------------------- SUMMARY MPBPWIN v1.40 --------------------
Vapor Pressure Estimations (25 deg C):
  (Using BP: 725.54 deg C (estimated))
  (Using MP: 317.95 deg C (estimated))
    VP:  8.95E-026 mm Hg (Antoine Method)
    VP:  1.73E-017 mm Hg (Modified Grain Method)
    VP:  8.8E-017 mm Hg (Mackay Method)
  Selected VP:  1.73E-017 mm Hg (Modified Grain Method)


HENRY (v3.10) Program Results:
============================

       Bond Est :  5.15E-014 atm-m3/mole
       Group Est:  Incomplete

SMILES : CCCCN(CCCC)(CC)CCCCCCN(CCCC)(CCCC)(CC)
CHEM   : BQAOH++  (twice charged form)
MOL FOR: C26 H58 N2
MOL WT : 398.77
------------------------- HENRYWIN v3.10 Results -------------------------
----------+-------------------------------------------+---------+----------
   CLASS  |     BOND CONTRIBUTION DESCRIPTION         | COMMENT |  VALUE
----------+-------------------------------------------+---------+----------
 HYDROGEN |  58  Hydrogen to Carbon (aliphatic) Bonds  |         | -6.9413
 FRAGMENT |  19  C-C                                   |         |  2.2098
 FRAGMENT |   8  C-N                                   |         | 10.4080
 FACTOR   |   *  Quaternary ammonium-type cmpd         | ESTIMATE|  6.0000
----------+-------------------------------------------+---------+----------
 RESULT   |    BOND ESTIMATION METHOD for LWAPC VALUE  |  TOTAL  | 11.676
----------+-------------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 5.15E-014 atm-m3/mole
                                = 2.11E-012 unitless


Henrys LC [VP/WSol estimate using EPI values]:
    HLC:  3.796E-021 atm-m3/mole
    VP:   1.73E-017 mm Hg
    WS:   2.39E+003 mg/L


ANION

MPBPWIN (v1.40) Program Results:
==============================
Experimental Database Structure Match:  no data
```

```
SMILES : CCOS(=O)(=O)O[Na]
CHEM   : Sodium monoethylsulfate
MOL FOR: C2 H5 O4 S1 Na1
MOL WT : 148.11
---------------------- SUMMARY MPBPWIN v1.40 --------------------


Boiling Point:  472.48 deg C (Adapted Stein and Brown Method)

Melting Point:  349.84 deg C (Adapted Joback Method)
Melting Point:  162.22 deg C (Gold and Ogle Method)
Mean Melt Pt :  256.03 deg C (Joback; Gold,Ogle Methods)
  Selected MP:  199.75 deg C (Weighted Value)

Vapor Pressure Estimations (25 deg C):
  (Using BP: 472.48 deg C (estimated))
  (Using MP: 199.75 deg C (estimated))
    VP:  7.11E-011 mm Hg (Antoine Method)
    VP:  1.94E-009 mm Hg (Modified Grain Method)
    VP:  5.33E-009 mm Hg (Mackay Method)
  Selected VP:  1.94E-009 mm Hg (Modified Grain Method)


HENRY (v3.10) Program Results:
==============================

       Bond Est :  1.08E-008 atm-m3/mole
       Group Est:  Incomplete

SMILES : CCOS(=O)(=O)O[Na]
CHEM   : Sodium monoethylsulfate
MOL FOR: C2 H5 O4 S1 Na1
MOL WT : 148.11
-------------------------- HENRYWIN v3.10 Results -------------------------
----------+-----------------------------------------+---------+----------
   CLASS  |     BOND CONTRIBUTION DESCRIPTION       | COMMENT |  VALUE
----------+-----------------------------------------+---------+----------
 HYDROGEN |   5  Hydrogen to Carbon (aliphatic) Bonds   |         | -0.5984
 FRAGMENT |   1  C-C                                |         |  0.1163
 FRAGMENT |   1  C-O                                |         |  1.0855
 FRAGMENT |   2  O-S                                | ESTIMATE|  0.4200
 FRAGMENT |   2  O=S (sulfone-type)                 | ESTIMATE|  2.1000
 FRAGMENT |   1  O-Na                               | ESTIMATE|  3.2300
----------+-----------------------------------------+---------+----------
 RESULT   |    BOND ESTIMATION METHOD for LWAPC VALUE   |  TOTAL  |  6.353
----------+-----------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 1.08E-008 atm-m3/mole
                                = 4.43E-007 unitless

--------+-----------------------------------------+------------+--------
        |       GROUP CONTRIBUTION DESCRIPTION    |   COMMENT  |  VALUE
--------+-----------------------------------------+------------+--------
        |          1  CH3 (X)                     |            | -0.62
        |          1  CH2 (C)(O)                  |            | -0.13
        |             MISSING Value for:  O (S)(C)
        |             MISSING Value for:  S (=O)(=O)(O)(O)
        |             MISSING Value for:  O (Na)(S)
        |             MISSING Value for:  UNTYPED(O)
--------+-----------------------------------------+------------+--------
 RESULT |  GROUP ESTIMATION METHOD for LOG GAMMA VALUE  | INCOMPLETE | -0.75
--------+-----------------------------------------+------------+--------


Henrys LC [VP/WSol estimate using EPI values]:
    HLC:  3.781E-016 atm-m3/mole
    VP:   1.94E-009 mm Hg
    WS:   1E+006 mg/L
```

Test substance :

BQAES CASNO 68052-49-3

Conclusion

The estimated vapor pressure is negligible at 2.2E-17 hPa for the cation and 2.6E-9 hPa for the anion.

Reliability : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag : Critical study for SIDS endpoint
02.01.2005 (3)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : at °C
pH value :
Method : other (calculated)
Year :
GLP :
Test substance : other TS

Method :

An octanol-water partition coefficient for the material was estimated using the KOWWIN program (v1.66) by entering the structure of the material into the program using SMILES code. This program estimates the partition coefficient by summing the coefficients of all fragments of the molecule based on an empirical equation that has been validated. As the material is a salt, independent calculations were conducted for the cation and anion.

Result :

KOWWIN Program (v1.66) Results:
==========

CATION Log Kow(version 1.66 estimate): 0.13

SMILES : CCCCN(CCCC)(CC)CCCCCCN(CCCC)(CCCC)(CC)
CHEM : BQAOH++ (charged form)
MOL FOR: C26 H58 N2
MOL WT : 398.77

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	6	-CH3 [aliphatic carbon]	0.5473	3.2838
Frag	20	-CH2- [aliphatic carbon]	0.4911	9.8220
Frag	2	>N< [+5 valence; single bonds;no H attach]	-6.6000	-13.2000
Const		Equation Constant		0.2290
			Log Kow =	0.1348

ANION Log Kow(version 1.66 estimate): -3.22

SMILES : CCOS(=O)(=O)O[Na]
CHEM : Sodium monoethylsulfate
MOL FOR: C2 H5 O4 S1 Na1
MOL WT : 148.11

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH3 [aliphatic carbon]	0.5473	0.5473
Frag	1	-CH2- [aliphatic carbon]	0.4911	0.4911
Frag	1	-O- [oxygen, aliphatic attach]	-1.2566	-1.2566
Frag	1	-O-SO2-O- [sulfate, linear]	1.3500	1.3500
Factor	1	S-O-{Na,K,Li} [coef*(1+0.3*(NUM-1))]	-4.5800	-4.5800
Const		Equation Constant		0.2290

Log Kow = -3.2192

Test substance :

BQAES CASNO 68052-49-3

Conclusion :

As the cationic material is a quaternary salt, it will remain charged at all pH values and will have an estimated log Kow of 0.13

As the anionic portion of the material is acidic, it will remain in the charged form at all but strongly acidic pH levels and is estimated to have a log Kow of -3.22 for the charged form.

Reliability : (2) valid with restrictions

Estimates conducted by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag : Critical study for SIDS endpoint
02.01.2005 (6)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : >= 480 g/l at 20 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: measured
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4

Method :

It is know from production of the material that solutions with content of 48% BQAES can be produced, stored and piped during production.

Conclusion :

This material is considered highly water soluble.

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint
02.01.2005 (7)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	
Rate constant	:	cm^3/(molecule*sec)
Degradation	:	% after

Method :

As this is an organic salt, it is necessary to consider both the cation and anion as the salt can easily dissociate

The structure was initially examined to determine if there was a chromophore that could absorb light energy at wavelengths above 295 um. As there is not for either cation or anion, it was assumed that direct photolysis would be unimportant to the fate of the test material.

The APOWIN program was also run to determine an estimated rate of reaction with hydroxyl radical. This rate was used to estimate the half-life of BQAOH in the troposphere assuming a tropospheric hydroxyl radical concentration of 1,500,000 molecules hydroxy radical per cm3.

Result :

AOP Program (v1.90) Results:
==========
SMILES : CCCCN(CCCC)(CC)CCCCCCN(CCCC)(CC)CCCC
CHEM : BQAOH
MOL FOR: C26 H58 N2
MOL WT : 398.77

```
--------------- SUMMARY (AOP v1.90): HYDROXYL RADICALS -------------------
Hydrogen Abstraction       =  98.3799 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   OVERALL OH Rate Constant =  98.3799 E-12 cm3/molecule-sec
   HALF-LIFE =     0.109 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE =     1.305 Hrs
```

AOP Program (v1.90) Results:
==========
SMILES : CCOS(=O)(=O)O[Na]
CHEM : Sodium monoethylsulfate
MOL FOR: C2 H5 O4 S1 Na1
MOL WT : 148.11

```
--------------- SUMMARY (AOP v1.90): HYDROXYL RADICALS -------------------
Hydrogen Abstraction       =   0.8211 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
```

```
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

  OVERALL OH Rate Constant =  0.8211 E-12 cm3/molecule-sec
  HALF-LIFE =    13.027 Days (12-hr day; 1.5E6 OH/cm3)
```

Test substance :

BQAES CASNO 68052-49-3

Conclusion :

Although vaporization into the atmosphere is considered unlikely, a value of approximately 1.3 hours is accepted as the atmospheric half-life of BQAES cation in the troposphere due to indirect photolysis and a value of approximately 13 days is accepted as the atmospheric half-life of BQAES anion in the troposphere due to indirect photolysis. No direct photolysis or reaction with atmospheric ozone is anticipated.

The calculated half-life of the cation is 1.3 hours based on 1,500,000 molecules of hydroxyl radical per cc.

The calculated half-life of the anion is 13 days based on 1,500,000 molecules of hydroxyl radical per cc.

Reliability : (2) valid with restrictions

Flag : Critical study for SIDS endpoint
02.01.2005 (2)

3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : at °C
t1/2 pH9 : at °C
Deg. product :
Method :
Year :
GLP :
Test substance : as prescribed by 1.1 - 1.4

Method :

Estimation on chemical principles for cation, literature value for anion.

Result :

The enthalpy of reaction for hydrolysis of quaternary amine to tertiary amine and alkyl alcohol is calculated by summing the strengths of bonds broken and subtracting the sum of the strengths of the bond formed. (Organic Chemistry by Peter Vollhardt, W.H. Freeman & Co, NY, NY 1987 pp71-73)

Bonds broken	
Water O-H	497 kJ
N-C	350 kJ

Bonds formed	
Alcohol C-OH	-356 kJ

Total estimated enthalpy of reaction = +491 kJ/mole

For the hydrolytic reaction of sodium ethyl sulfate, standard bond energies are not available for the sulfur-oxygen bond in sulfate and the organic ester. Examination of the structure suggests that hydrolysis may occur at a reasonable rate. The hydrolysis rate of diethyl sulfate to ethanol and sulfate has been determined to be 1.15X10-4/sec at 25 deg C (Can J Chem 44: 1728-30,1966 as cited in HSBD) translates to a half-life of 1.7 hours at pH 7(SRC, as cited in HSDB). The rate of hydrolysis will increase in both acidic and basic waters as the reaction is catalyzed under these conditions (Weisenberger K, Mayer D; Ullmann's Encycl Indust Chem. MY, NY: VCH Pub A8: 493-504 1987, as cited in HSDB). Although the hydrolysis rate of diethyl sulfate comprises two hydrolytic reactions, a half life of hours for the overall reaction indicates a half-life of less than 1 day for sodium ethyl sulfate.

Bond energies from Lide, Handbook of Chemistry 84th edition 2003-2004 section 9

Conclusion :

The hydrolysis of the quaternary nitrogen to a tertiary amine and an alcohol is thermodynamically very unfavorable with a delta G estimated from the delta H of reaction greater than +400 kJ/mole. This is predicted to be a very endothermic reaction and should occur only under conditions of very high temperature.

It can be concluded that the quaternary amine portion of BQAES is stable in water and has a hydrolysis half-life of greater than 1 year.

The ethyl sulfate anion will hydrolyze readily and is estimated to have a half-life of less than 1 day in the environment.

Reliability : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag : Critical study for SIDS endpoint
03.01.2005 (5)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : other: air water soil sedement
Method : Calculation according Mackay, Level III
Year :

Method :

Theoretical Distribution (Fugacity) of BQAES in the environment was estimated using the MacKay EQC level III model set to estimate distribution after equal release to water, air and soil. The EPIWIN model was allowed to estimate physicochemical and fate parameters used in the calculations; however, these were verified for appropriateness before the final calculation was accepted. Because BQAES is a salt and is expected to dissociate in the environment, the cationic and anionic portions of the salt were independently modeled

Result :

Level III Fugacity Model (Full-Output):

```
  Chem Name   : BQAOH and BQAES Cation
  Molecular Wt: 398.77
  Henry's LC  : 5.15e-014 atm-m3/mole (Henrywin program)
  Vapor Press : 1.73e-017 mm Hg  (Mpbpwin program)
  Liquid VP   : 1.37e-014 mm Hg  (super-cooled)
  Melting Pt  : 318 deg C (Mpbpwin program)
  Log Kow     : 0.13  (Kowwin program)
  Soil Koc    : 0.553  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       1.72e-010       2.61         0
   Water     99.8            208          1000
   Soil      1.15e-009       208          0
   Sediment  0.15            832          0

     Fugacity   Reaction   Advection  Reaction   Advection
       (atm)     (kg/hr)    (kg/hr)   (percent)  (percent)
Air   3.69e-030  1.05e-007 3.97e-009  1.05e-008  3.97e-010
Water 1.49e-019  769       231        76.9       23.1
Soil  6.09e-029  8.86e-009  0         8.86e-010   0
Sedi  1.11e-019  0.29      0.00696    0.029      0.000696

   Persistence Time: 231 hr
   Reaction Time:    301 hr
   Advection Time:   1e+003 hr
   Percent Reacted:  76.9
   Percent Advected: 23.1

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      2.609
      Water:    208.1
      Soil:     208.1
      Sediment: 832.3
        Biowin estimate: 3.511  (days-weeks  )

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004



Level III Fugacity Model (Full-Output):
  Chem Name   : Sodium monoethylsulfate
  Molecular Wt: 148.11
  Henry's LC  : 1.08e-008 atm-m3/mole (Henrywin program)
  Vapor Press : 1.94e-009 mm Hg  (Mpbpwin program)
  Liquid VP   : 1.04e-007 mm Hg  (super-cooled)
  Melting Pt  : 200 deg C (Mpbpwin program)
  Log Kow     : -3.22  (Kowwin program)
  Soil Koc    : 0.000247  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.000177        313          0
```

```
   Water     99.8           360          1000
   Soil      0.00289        360          0
   Sediment  0.166          1.44e+003    0

      Fugacity   Reaction Advecti  Reaction  Advection
       (atm)     (kg/hr)   (kg/hr) (percent) (percent)
Air   1.03e-016  0.00134  0.00605  0.000134  0.000605
Water 1.25e-013  658      342      65.8      34.2
Soil  1.34e-016  0.0191   0        0.00191   0
Sedi  1.04e-013  0.274    0.0114   0.0274    0.00114

   Persistence Time: 342 hr
   Reaction Time:    520 hr
   Advection Time:   1e+003 hr
   Percent Reacted:  65.8
   Percent Advected: 34.2

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      312.7
      Water:    360
      Soil:     360
      Sediment: 1440
        Biowin estimate: 2.872  (weeks)

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004
```

Test substance :

BQAES CASNO 68052-49-3

Conclusion :

If released into water, the material remains primarily in the water column.

Reliability : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag : Critical study for SIDS endpoint

04.01.2005 (3)

3.5 BIODEGRADATION

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

5.1.1 ACUTE ORAL TOXICITY

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

5.5 GENETIC TOXICITY ‘IN VITRO‘

5.6 GENETIC TOXICITY ‘IN VIVO‘

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

(1) Calculated by Toxicology and Regulatory Affairs, December 2004.

(2) Calculated using EPIWIN 3.05 by Toxicology and Regulatory Affairs, December 2004

(3) Calculated using EPIWIN 3.05 by Toxicology and Regulatory Affairs, December 2004

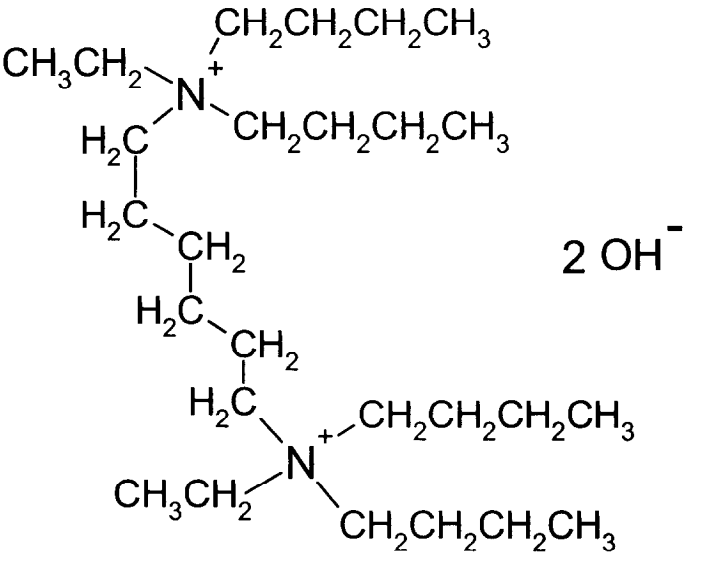
(4) Calculated using MPBPWIN (v1.40) Program as found in EPIWIN 3.05 (2000, EPA version) by Toxicology and Regulatory Affairs, December 2004

(5) Estimation conducted by Toxicology and Regulatory Affairs, December 2004.

(6) Estimation conducted using KOWWIN Program (v1.66) as found in EPIWIN 3.05, Syracuse Research Corporation, ES EPA Version 2000, calculation by Toxicology and Regulatory Affairs, December 2004.

(7) Solitia MSDS #068052493 for BQAES 45 - 97 % Aqueous Solution. 21 September 1998.

HPV Data Set



BQAOH

Existing Chemical	:	ID: 111960-92-0
CAS No.	:	111960-92-0
Product name	:	BQAOH
TSCA Name	:	1,6-Hexanediaminium, N,N,N',N'-tetrabutyl-N,N'-diethyl-,dihydroxide
Producer related part		
Company	:	Solutia Inc
Creation date	:	10.01.2004
Substance related part		
Company	:	Toxicology and Regulatory Affairs
Creation date	:	10.01.2004
Status	:	
Memo	:	Prepared by: Toxicology and Regulatory Affairs Freeburg IL 62243 rauckman@toxicsolutions.com
Printing date	:	09.01.2005
Revision date	:	
Date of last update	:	04.01.2005
Number of pages	:	22
Chapter (profile)	:	
Reliability (profile)	:	
Flags (profile)	:	

1.0.1 APPLICANT AND COMPANY INFORMATION

Type	:	manufacturer
Name	:	Solutia Inc
Contact person	:	
Date	:	
Street	:	
Town	:	
Country	:	
Phone	:	
Telefax	:	
Telex	:	
Cedex	:	
Email	:	
Homepage	:	

10.01.2004

1.2 SYNONYMS AND TRADENAMES

2.1 MELTING POINT

Value	:	ca. 0 - -3.2 °C
Sublimation	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4
Method	:	The material as produced is an aqueous solution containing up to 25% BQAOH. The practical freezing point of the solution is a function of the solvent's freezing point and the freezing point depression caused by the solute. An approximate freezing point can be calculated based on the molal freezing-point depression constant for water of 1.86°C
Result	:	For a 25% solution of BQAOH in water the approximate molality is 0.577. Considering that there could be up to three ions, the freezing point depression could be as great as 3.21°C.
Conclusion	:	The freezing point range for this material as an aqueous solution is 0 to -3.2°C; however, limits on the solubility could cause precipitated solid formation prior to freezing.
Reliability	:	(2) valid with restrictions Estimates calculated by a reliable method are assigned a reliability score of 2.
Flag	:	Critical study for SIDS endpoint
10.01.2004		

Value	:	<= 380 °C
Sublimation	:	
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS
Method	:	This material is produced, handled and disposed of as an aqueous solution containing up to 25% organic content. The melting point for the solid material has not been recorded as it is not isolated, but as an impure salt it is expected to be relatively high and variable. For the purpose of an HPV program, the melting point of the solid was estimated with the MPBPWIN (v 1.4) program. This estimate is considered an upper limit of the practical melting point for the solid.
Result	:	MPBPWIN (v1.40) Program Results: ========== Experimental Database Structure Match: no data SMILES : CCCCN(CCCC)(CC)CCCCCCN(CCCC)(CCCC)(CC) CHEM : BQAOH++ (twice charged form) MOL FOR: C26 H58 N2 MOL WT : 398.77

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	6	-CH3	-5.10	-30.60
Group	20	-CH2-	11.27	225.40
Group	2	>N< (+5)	340.00	680.00
*		Equation Constant		122.50
RESULT		MELTING POINT in deg Kelvin		997.30
RESULT-limit		MELTING POINT in deg Kelvin		623.00
		MELTING POINT in deg C		349.84

Melting Point: 349.84 deg C (Adapted Joback Method)
Melting Point: 309.98 deg C (Gold and Ogle Method)
Mean Melt Pt : 329.91 deg C (Joback; Gold,Ogle Methods)
Selected MP: 317.95 deg C (Weighted Value)

Test substance :

Solid portion of BQAOH solution as produced.

Conclusion :

The actual melting point of the solid portion of this material is expected to vary, depending on the impurity level, with a maximum of 318 °C

Reliability : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2.

Flag : Critical study for SIDS endpoint

02.01.2005 (10)

2.2 BOILING POINT

Value : ca. 100 - 101 °C at 1013 hPa

Decomposition :

Method : other: calculated

Year :

GLP :

Test substance : as prescribed by 1.1 - 1.4

Method :

The material as produced is an aqueous solution containing up to 25% BQAOH. The practical boiling point of the solution is a function of the solvent's boiling point and the boiling point elevation caused by the solute. An approximate boiling point can be calculated based on the molal boiling-point elevation constant for water of 0.52°C/m.

Remark :

The solid material is expected to decompose before boiling as it is a high molecular weight salt.

Result :

For a 25% solution of BQAOH in water, the approximate molality is 0.577. Considering that there could be up to three ions, the boiling-point elevation could be as great as 0.9°C.

Conclusion :

The initial boiling point range for this material as an aqueous solution is 100

to 101°C.

Reliability : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2.

Flag : Critical study for SIDS endpoint
10.01.2004

2.3 DENSITY

2.4 VAPOUR PRESSURE

Value : < .000000000001 hPa at 25 °C
Decomposition :
Method : other (calculated): EPIWIN
Year :
GLP :
Test substance : other TS

Method :

The vapor pressure for a charged salt is expected to be negligible. In addition, as this material is produced and handled as an aqueous solution, the Henry's law constant is a more important factor for exposure consideration from bulk material or material that is introduced into the water column. EPIWIN was used to provide estimates for both the vapor pressure and the Henry's law constant. EPIWIN was also used to estimate the half live for volatilization from water in a model river.

Result :

MPBPWIN (v1.40) Program Results:
==========
Experimental Database Structure Match: no data

```
SMILES : CCCCN(CCCC)(CC)CCCCCCN(CCCC)(CCCC)(CC)
CHEM   : BQAOH++  (twice charged form)
MOL FOR: C26 H58 N2
MOL WT : 398.77
---------- SUMMARY MPBPWIN v1.40 ----------
Vapor Pressure Estimations (25 deg C):
  (Using BP: 725.54 deg C (estimated))
  (Using MP: 317.95 deg C (estimated))
    VP:  8.95E-026 mm Hg (Antoine Method)
    VP:  1.73E-017 mm Hg (Modified Grain Method)
    VP:  8.8E-017 mm Hg (Mackay Method)
  Selected VP:  1.73E-017 mm Hg (Modified Grain Method)
```

```
HENRY (v3.10) Program Results:
==========

       Bond Est :  5.15E-014 atm-m3/mole
       Group Est:  Incomplete

SMILES : CCCCN(CCCC)(CC)CCCCCCN(CCCC)(CCCC)(CC)
CHEM   : BQAOH++  (twice charged form)
MOL FOR: C26 H58 N2
MOL WT : 398.77
```

```
--------------------------- HENRYWIN v3.10 Results --------------------------
----------+-----------------------------------------+---------+----------
   CLASS  |     BOND CONTRIBUTION DESCRIPTION       | COMMENT |  VALUE
----------+-----------------------------------------+---------+----------
 HYDROGEN |  58  Hydrogen to Carbon (aliphatic) Bonds   |         | -6.9413
 FRAGMENT |  19  C-C                                |         |  2.2098
 FRAGMENT |   8  C-N                                |         | 10.4080
 FACTOR   |   *  Quaternary ammonium-type cmpd      | ESTIMATE|  6.0000
----------+-----------------------------------------+---------+----------
 RESULT   |    BOND ESTIMATION METHOD for LWAPC VALUE   |  TOTAL  | 11.676
----------+-----------------------------------------+---------+----------
HENRYs LAW CONSTANT at 25 deg C = 5.15E-014 atm-m3/mole
                               = 2.11E-012 unitless


Henrys LC [VP/WSol estimate using EPI values]:
    HLC:  3.796E-021 atm-m3/mole
    VP:   1.73E-017 mm Hg
    WS:   2.39E+003 mg/L


---------------VOLATIZATION FROM WATER-------------

                             RIVER            LAKE
                           ---------        ---------
Water Depth     (meters):   1                1
Wind Velocity    (m/sec):   5                0.5
Current Velocity (m/sec):   1                0.05

      HALF-LIFE (hours) :   2.27E+010        2.477E+011
      HALF-LIFE (days ) :   9.459E+008       1.032E+010
      HALF-LIFE (years) :   2.59E+006        2.825E+007
```

Test substance :

Solid portion of BQAOH solution as produced.

Conclusion

The estimated vapor pressure is negligible at 2.2E-17 hPa

Reliability : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2.

Flag : Critical study for SIDS endpoint

10.01.2004 (11)

2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : ca. .13 at 25 °C
pH value :
Method : other (calculated): EPIWIN
Year :
GLP :
Test substance : other TS

Method :

An octanol-water partition coefficient for the material was estimated using the KOWWIN program (v1.66) by entering the structure of the material into the program using SMILES code. This program estimates the partition coefficient by summing the coefficients of all fragments of the molecule based on an empirical equation that has been validated.

Result : KOWWIN Program (v1.66) Results:
==========

Log Kow(version 1.66 estimate): 0.13

SMILES : CCCCN(CCCC)(CC)CCCCCCN(CCCC)(CCCC)(CC)
CHEM : BQAOH++ (charged form)
MOL FOR: C26 H58 N2
MOL WT : 398.77

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	6	-CH3 [aliphatic carbon]	0.5473	3.2838
Frag	20	-CH2- [aliphatic carbon]	0.4911	9.8220
Frag	2	>N< [+5 valence; single bonds;no H attach]	-6.6000	-13.2000
Const		Equation Constant		0.2290

Log Kow = 0.1348

Test substance :

BQAOH CASNO 111960-92-0 (as smiles notation)

Conclusion :

As the cationic material is a quaternary salt, it will remain charged at all pH values and will have an estimated log Kow of 0.13

Reliability : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag : Critical study for SIDS endpoint
02.01.2005 (8)

2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : >= 280 g/l at 20 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description : very soluble (> 10000 mg/L)
Stable :

Remark :

It is know from production and testing of the material that solutions with content of 28 % BQAOH can be produced and shipped for toxicity testing. In addition the MSDS specification allows for solutions concentrated as 25% by weight.

Conclusion :

This material is considered highly water soluble.

Reliability : (2) valid with restrictions

Information obtained by a scientifically defensible method.

Flag : Critical study for SIDS endpoint
10.01.2004 (9)

3.1.1 PHOTODEGRADATION

Type	:	air
Light source	:	Sun light
Light spectrum	:	nm
Relative intensity	:	based on intensity of sunlight
DIRECT PHOTOLYSIS		
Halflife t1/2	:	ca. 1.3 hour(s)
Degradation	:	% after
Quantum yield	:	
INDIRECT PHOTOLYSIS		
Sensitizer	:	OH
Conc. of sensitizer	:	
Rate constant	:	cm^3/(molecule*sec)
Degradation	:	% after

Method :

The structure was initially examined to determine if there was a chromophore that could absorb light energy at wavelengths above 295 um. As there is not, it was assumed that direct photolysis would be unimportant to the fate of the test material.

The APOWIN program was also run to determine an estimated rate of reaction with hydroxyl radical. This rate was used to estimate the half-life of BQAOH in the troposphere assuming a tropospheric hydroxyl radical concentration of 1,500,000 molecules hydroxy radical per cm3.

Result :

The calculated half-life is 1.3 hours based on 1,500,000 molecules of hydroxyl radical per cc.

AOP Program (v1.90) Results:

```
==========================
SMILES : CCCCN(CCCC)(CC)CCCCCCN(CCCC)(CC)CCCC
CHEM   : BQAOH
MOL FOR: C26 H58 N2
MOL WT : 398.77
------------ SUMMARY (AOP v1.90): HYDROXYL RADICALS ------------------
Hydrogen Abstraction       =  98.3799 E-12 cm3/molecule-sec
Reaction with N, S and -OH =   0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds   =   0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds =   0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings =   0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec
```

OVERALL OH Rate Constant = 98.3799 E-12 cm3/molecule-sec
HALF-LIFE = 0.109 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 1.305 Hrs

Conclusion :

Although vaporization into the atmosphere is considered unlikely, a value of approximately 1.3 hours is accepted as the atmospheric half-life of BQAOH in the troposphere due to indirect photolysis. No direct photolysis or reaction with atmospheric ozone is anticipated.

Reliability : (2) valid with restrictions
Flag : Critical study for SIDS endpoint
02.01.2005 (3)

3.1.2 STABILITY IN WATER

Type	:	abiotic
t1/2 pH4	:	at °C
t1/2 pH7	:	at °C
t1/2 pH9	:	at °C
Deg. product	:	
Method	:	
Year	:	
GLP	:	
Test substance	:	as prescribed by 1.1 - 1.4

Method :

Estimation on chemical principles.

Result :

The enthalpy of reaction for hydrolysis of quaternary amine to tertiary amine and alkyl alcohol is calculated by summing the strengths of bonds broken and subtracting the sum of the strengths of the bond formed. (Organic Chemistry by Peter Vollhardt, W.H. Freeman & Co, NY, NY 1987 pp71-73)

Bonds broken

Water O-H	497 kJ
N-C	350 kJ

Bonds formed

Alcohol C-OH	-356 kJ

Total estimated enthalpy of reaction = +491 kJ/mole

Bond energies from Lide, Handbook of Chemistry 84th edition 2003-2004 section 9

Conclusion :

The hydrolysis of the quaternary nitrogen to a tertiary amine and an alcohol is thermodynamically very unfavorable with a delta G estimated from the delta H of reaction to be greater than +400 kJ/mole. This is predicted to be a very endothermic reaction and should occur only under conditions of very high temperature.

It can be concluded that the quaternary amine portion of BQAOH is stable in water and has a hydrolysis half-life of greater than 1 year.

Reliability : (2) valid with restrictions

Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).

Flag : Critical study for SIDS endpoint

02.01.2005 (2)

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : other: air water soil sedement
Method : Calculation according Mackay, Level III
Year :

Method :

Theoretical Distribution (Fugacity) of BQAOH in the environment was estimated using the MacKay EQC level III model set to estimate distribution after equal release to water, air and soil. The EPIWIN model was allowed to estimate physicochemical and fate parameters used in the calculations; however, these were verified for appropriateness before the final calculation was accepted. Because BQAOH is a salt and is expected to dissociate in the environment, the cationic portions were independently modeled.

Result :

Level III Fugacity Model (Full-Output):

```
=====================================
  Chem Name   : BQAOH and BQAES Cation
  Molecular Wt: 398.77
  Henry's LC  : 5.15e-014 atm-m3/mole (Henrywin program)
  Vapor Press : 1.73e-017 mm Hg  (Mpbpwin program)
  Liquid VP   : 1.37e-014 mm Hg  (super-cooled)
  Melting Pt  : 318 deg C (Mpbpwin program)
  Log Kow     : 0.13  (Kowwin program)
  Soil Koc    : 0.553  (calc by model)

          Concentration   Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       1.72e-010       2.61         0
   Water     99.8            208          1000
   Soil      1.15e-009       208          0
   Sediment  0.15            832          0

      Fugacity   Reaction   Advection  Reaction   Advection
        (atm)     (kg/hr)    (kg/hr)   (percent)  (percent)
Air   3.69e-030  1.05e-007 3.97e-009  1.05e-008  3.97e-010
Water 1.49e-019  769       231        76.9       23.1
Soil  6.09e-029  8.86e-009  0         8.86e-010   0
Sedi  1.11e-019  0.29      0.00696    0.029      0.000696

   Persistence Time: 231 hr
   Reaction Time:    301 hr
   Advection Time:   1e+003 hr
   Percent Reacted:  76.9
   Percent Advected: 23.1

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      2.609
      Water:    208.1
      Soil:     208.1
      Sediment: 832.3
        Biowin estimate: 3.511  (days-weeks  )

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004
```

Test substance	:	BQAOH CASNO 111960-92-0 (as smiles notation)
Conclusion	:	If released into water, the material remains primarily in the water column.
Reliability	:	(2) valid with restrictions Estimates calculated by a reliable method are assigned a reliability score of 2 (reliable with restrictions).
Flag	:	Critical study for SIDS endpoint

04.01.2005 (4)

3.5 BIODEGRADATION

4.1 ACUTE/PROLONGED TOXICITY TO FISH

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

5.1.1 ACUTE ORAL TOXICITY

Type	:	LD50
Value	:	= 350 mg/kg bw
Species	:	rat
Strain	:	Sprague-Dawley
Sex	:	male/female
Number of animals	:	
Vehicle	:	other: Dosed as produced (28% solution in water)
Doses	:	
Method	:	
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Method :

Groups of five young adult Sprague-Dawley male rats of each sex were administered test material by intragastric intubation as received. The test material was accompanied by a sample identification sheet specifying that the test material was "28% pure". It is assumed that the remainder was water, consistent with the product description in other literature. At dosing, average group weight of males was 200 to 220 g and average group weight of females was 185-210 grams. Surviving animals were observed for 14 days and were sacrificed and necropsied.

Result :

Dose levels and results are given in the table

MALES

Dose 28% soln	As BQAOH	Mortality	Time of Death
2,000	560	5/5	30 -120 min
1,580	442	4/5	30 -120 min
1,260	315	2/5	120 min
1,000	280	1/5	30 min
794	222	0/5	-

FEMALES

Dose 28% soln	As BQAOH	Mortality	Time of Death
2,000	560	5/5	30 -120 min
1,580	442	5/5	120 min
1,260	315	4/5	30 - 120 min
1,000	280	1/5	120 min
794	222	0/5	-

CLINICAL EFFECTS:

@ Lethal Doses: Lethargy, rapidly increasing weakness, collapse and death.

@ Nonlethal Doses: Lethargy lasting 1 day.

GROSS NECROPSY FINDINGS

Decedents: Hemorrhagic lung and liver, liver discoloration in some cases, one animal showed kidney discoloration, gastrointestinal inflammation.

Survivors: Viscera appeared normal at sacrifice.

Conclusion :

BQAOH has an acute oral LD50 in Sprague-Dawley rats of 1250 mg/kg (95% CI 1120- 1380) based on the 28% solution. As a pure material it has an LD50 of 350 mg/kg (95% CI 314-386). Male and female rats are approximately equally sensitive.

Reliability : (1) valid without restriction

Study protocol was comparable to current OECD guideline, study conducted under GLP.

Flag : Critical study for SIDS endpoint
24.01.2004 (14)

5.1.2 ACUTE INHALATION TOXICITY

5.1.3 ACUTE DERMAL TOXICITY

Type	:	LD50
Value	:	= 22.4 mg/kg bw
Species	:	rabbit
Strain	:	New Zealand white
Sex	:	male/female
Number of animals	:	
Vehicle	:	other: Applied as produced (28% water solution)
Doses	:	
Method	:	
Year	:	
GLP	:	yes
Test substance	:	as prescribed by 1.1 - 1.4

Method :

Groups of two New Zealand albino rabbits of each sex were dermally exposed to undiluted test material at 6 closely spaced dose levels. At each dose level, one animal's skin was abraded and the other's skin was left intact. The test material remained in contact with the skin for 24 hours and was then removed.

The test material was accompanied by a sample identification sheet specifying that the test material was "28% pure". It is assumed that the remainder was water, consistent with the description of the product in other literature. Surviving animals were observed for 14 days then were sacrificed and necropsied.

Result :

Dose levels and mortality results are given in the table

MALES

Dose 28% soln	As BQAOH	Mortality intact	Mortality abraded	Time of Death
50.1	14.0	0/1	0/1	-
63.1	17.7	1/1	0/1	2 hours
79.4	22.2	0/1	0/1	-
100.0	28.0	1/1	1/1	2 hours
126.0	35.3	1/1	1/1	2 hours
158.0	44.2	1/1	1/1	2 hours

FEMALES

Dose 28% soln	As BQAOH	Mortality intact	Mortality abraded	Time of Death
50.1	14.0	0/1	0/1	-
63.1	17.7	0/1	1/1	24 hours
79.4	22.2	1/1	0/1	2 hours
100.0	28.0	1/1	1/1	2 hours
126.0	35.3	0/1	1/1	2 hours
158.0	44.2	1/1	1/1	2 hours

CLINICAL EFFECTS:

@ Lethal Doses: Rapidly increasing weakness, collapse and death.

@ Nonlethal Doses: Not reported.

GROSS NECROPSY FINDINGS

Decedents: Hemorrhagic areas of lung, liver discoloration in one animal, two animals showed enlarged gall bladders.

Survivors: Viscera appeared normal at sacrifice.

Conclusion :

BQAOH is very toxic to rabbits by the dermal route with an acute dermal LD50 in rabbits of 80 mg/kg (95% CI 67 - 94) based on the 28% solution. As a pure material it has an LD50 of 22.4 mg/kg (95% CI 18.8 - 26.3). Males and females have approximately equal sensitivity.

Reliability : (1) valid without restriction

Although the number of animals per group was low, sufficient data were generated by a scientifically defensible method, using GLP conditions, to consider this a reliable estimate of dermal toxicity.

Flag : Critical study for SIDS endpoint

24.01.2004 (14)

5.1.4 ACUTE TOXICITY, OTHER ROUTES

5.4 REPEATED DOSE TOXICITY

Type	:	Chronic
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	104 Weeks
Frequency of treatm.	:	Cont
Post exposure period	:	
Doses	:	300, 750 or 1500 ppm
Control group	:	yes, concurrent vehicle
NOAEL	:	= 750 ppm
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS

Method :

Test substance was fed in diet to 60 Sprague-Dawley CD rats/sex/group for 104 weeks at 0 (Ground Purina Certified Rodent Chow # 5002), 300, 750, or 1500 ppm. Two control groups were included and treated as independent entities.

Result :

Chronic NOEL = 750 ppm (Decreased bodyweight, bodyweight gain and food consumption was observed in each sex at 1500 ppm. Increased incidence in mesenteric lymph node pathology (blood in sinuses, hemosiderosis and histiocytosis) occurred in both sexes at 1500 ppm. Bile duct hyperplasia occurred in females at 1500 ppm.) Treatment-related oncogenicity was not observed. No adverse oncogenic effects were observed, however, there were treatment-related changes in both sexes in the mesenteric lymph node (blood filled sinuses, hemosiderosis & hystiocytosis) and bile duct hyperplasia at 1500 ppm.

Test substance :

Bardac 2280 (didecyldimethylammonium chloride, CASNO 7173-51-5), 80.8% pure

Reliability : (2) valid with restrictions

Study judged as "acceptable" by California EPA for establishing pesticide tolerance

Flag : Critical study for SIDS endpoint

04.01.2005 (6)

5.5 GENETIC TOXICITY 'IN VITRO'

Type	:	HGPRT assay
System of testing	:	CHO Cells
Test concentration	:	
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	
Year	:	

GLP	:	no data
Test substance	:	other TS
Method	:	Test material was assayed in a CHO/HGPRT forward mutation assay at concentrations of 0 (vehicle = deionized water), 3.0, 4.0, 5.0, 6.0, 7.0, 8.0 and 10.0 µg/ml without metabolic activation.
Result	:	In the first trial, the survival ranged from 105.9% to 10.7%. The second trial gave survivals ranging from 106.6% to 5.7%. Neither assay showed an increase in mutant frequency. Trials with metabolic activation were conducted at concentrations of 0, 1.0, 5.0, 10.0, 13.0, 15.0, 18.0, 20.0, 22.0 and 25.0 µg/ml. The first trial yielded survivals of 105.1% to 2.8% (at doses from 5.0 to 25.0 µg/ml). The repeat trial yielded survivals from 102.4% to 19.3% (at doses from 10.0 to 22.0 µg/ml). Neither trial showed an increase in mutant frequency.
Test substance	:	Bardac 2280 (didecyldimethylammonium chloride, CASNO 7173-51-5), 80% B-1889
Reliability	:	(2) valid with restrictions Study judged as "acceptable" by California EPA for establishing pesticide tolerance
Flag	:	Critical study for SIDS endpoint

04.01.2005 (12)

Type	:	Cytogenetic assay
System of testing	:	CHO Cells
Test concentration	:	
Cycotoxic concentr.	:	
Metabolic activation	:	with and without
Result	:	negative
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS
Method	:	A 50% solution of didecyldimethylammonium chloride was tested in an in vitro cytogenetic assay in the presence of activation (+S9) with Chinese Hamster ovary cells in duplicate at concentrations of untreated, 0 (deionized distilled water), 2, 4, 8, and 16 µg/ml. In the absence of activation (no S9), concentrations for the first replicate were untreated, 0 (deionized distilled water), 0.25, 0.5, 1.0, and 2.0 µg/ml. These levels did not produce the expected toxicity and levels for the second replicate were increased to: untreated, 0, 1.0, 2.0, 4.0, and 8.0 µg/ml.
Result	:	No adverse effects either with or without S9
Test substance	:	Bardac 2280 (didecyldimethylammonium chloride, CASNO 7173-51-5), 50% in water tested as PO151
Reliability	:	(2) valid with restrictions Study judged as "acceptable" by California EPA for establishing pesticide tolerance
Flag	:	Critical study for SIDS endpoint

04.01.2005 (5)

5.6 GENETIC TOXICITY 'IN VIVO'

Type	:	Cytogenetic assay
Species	:	rat
Sex	:	male/female
Strain	:	Crj: CD(SD)
Route of admin.	:	gavage
Exposure period	:	6, 24 or 48 hours
Doses	:	600 mg/kg
Result	:	negative
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS

Method :

The test substance was administered by gavage to CD albino rats (5/sex/sampling time) at 0 (distilled water) and 600 mg/kg. Bone marrow sampling of vehicle control and test substance groups was performed at 6, 24, and 48 hours. The positive control, cyclophosphamide (40 mg/kg), was sampled at 24 hours.

Result :

No treatment-related effects to metaphase chromosomes were observed.

Positive controls gave the expected result.

Test substance :

Didecyldimethylammonium chloride, CASNO 7173-51-5, 50.3% solution

Reliability : (2) valid with restrictions

Study judged as "acceptable" by California EPA for establishing pesticide tolerance

Flag : Critical study for SIDS endpoint

04.01.2005 (1)

5.8.1 TOXICITY TO FERTILITY

Type	:	Two generation study
Species	:	rat
Sex	:	male/female
Strain	:	Sprague-Dawley
Route of admin.	:	oral feed
Exposure period	:	
Frequency of treatm.	:	Cont
Premating exposure period		
Male	:	10 weeks
Female	:	10 weeks
Duration of test	:	
No. of generation studies	:	2
Doses	:	300, 750 or 1500 ppm
Control group	:	yes, concurrent vehicle
NOAEL parental	:	= 750 ppm

NOAEL F1 offspring	:	= 750 ppm
NOAEL F2 offspring	:	= 750 ppm
Result	:	Not a specific reproductive toxin
Method	:	
Year	:	
GLP	:	no data
Test substance	:	other TS

Method :

Didecyldimethylammoniumchloride (80.8% pure), was fed in diet to Sprague-Dawley (CD) rats (28/sex/dose) through two generations with 2 litters per generation at 0 (Purina Certified Ground Rodent Chow. #5002),300, 750, or 1500 ppm. Treatment began 10 weeks prior to mating.

:

Result

Parental NOEL = 750 ppm (Reduced bodyweights and food consumption were observed at 1500 ppm).

Reproductive NOEL = 750 ppm (Pups had reduced bodyweight gain at 1500 ppm).

Test substance :

Didecyldimethylammoniumchloride, CASNO 7173-51-5 (80.8% pure)

Reliability : (2) valid with restrictions

Study judged as "acceptable" by California EPA for establishing pesticide tolerance

Flag : Critical study for SIDS endpoint

04.01.2005 (13)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species	:	rabbit
Sex	:	
Strain	:	New Zealand white
Route of admin.	:	gavage
Exposure period	:	day 6 - 18 of gestation
Frequency of treatm.	:	daily
Duration of test	:	
Doses	:	1, 3 or 10 mg/kg-day
Control group	:	yes, concurrent vehicle
NOAEL maternal tox.	:	= 1 mg/kg bw
NOAEL teratogen.	:	mg/kg bw
other: NOEL	:	= 3
Developmental		

Method :

Test material was administered by gavage to mated New Zealand White rabbits on days 6 - 18 of gestation (day of mating = day 0 of gestation) at 0 (vehicle = deionized water), 1.0, 3.0 or 10.0 mg/kg/day (16/group).

Result :

Maternal NOEL = 1.0 mg/kg (4 deaths accompanied by labored respiration, gasping, sloughing of esophageal lining and stomach, and decreased weight gain was observed at 10.0 mg/kg. At 3.0 mg/kg audible respiration, hypoactivity and decreased weight gain was observed.)

Developmental NOEL = 3.0 mg/kg (An increased number of dead fetuses/litter and decreased fetal body weight at 10.0 mg/kg was observed.)

Test substance :

Bardac 2280 (didecyldimethylammonium chloride, CASNO 7173-51-5), 80.8% pure, Batch B-1889

Reliability : (2) valid with restrictions

Study judged as "acceptable" by California EPA for establishing pesticide tolerance

Flag : Critical study for SIDS endpoint

04.01.2005 (7)

(1) Analysis of Metaphase Chromosomes Obtained from Bone Marrow of Rats Treated with P0151", (J.A. Allen, R.J. Proudlock & P.C. Brooker, Huntingdon Research Center, Huntingdon, England, Project # LZA 24/8761, 4/1/87). As cited in; California EPA Dept of Pesticide Regulation Medical Toxicology Branch. Summary of Toxicology Data Didecyldimehylammoniumchloride revised 2/14/1996. http://www.cdpr.ca.gov/docs/toxsums/pdfs/1682.pdf

(2) Calculated by Toxicology and Regulatory Affairs, December 2004

(3) Calculated using EPIWIN 3.05 by Toxicology and Regulatory Affairs, October 2004

(4) Calculated using EPIWIN 3.05 by Toxicology and Regulatory Affairs, October 2004

(5) Chromosomal Aberrations Assay with Chinese Hamster Ovary Cells in vitro", (M. Holmstrom, D.J. Leftwich & I.A. Leddy, Gulland Laboratories of Inveresk Research International, Musselburgh, Scotland, Report # 4236, October 1986). As cited in; California EPA Dept of Pesticide Regulation Medical Toxicology Branch. Summary of Toxicology Data Didecyldimehylammoniumchloride revised 2/14/1996. http://www.cdpr.ca.gov/docs/toxsums/pdfs/1682.pdf

(6) Chronic Dietary Toxicity/Oncogenicity Study with Didecyldimethylammoniumchloride in Rats", (M.W. Gill, J.S. Chun & C.L. Wagner, Bushy Run Research Center, Export, PA., Report # 53-566, 6/27/91). As cited in; California EPA Dept of Pesticide Regulation Medical Toxicology Branch. Summary of Toxicology Data Didecyldimehylammoniumchloride revised 2/14/1996. http://www.cdpr.ca.gov/docs/toxsums/pdfs/1682.pdf

(7) Developmental Toxicity Study of Didecyldimethyl ammonium chloride Administered by Gavage to New Zealand White Rabbits," (Tyl, R.W., Bushy Run Research Center, Project ID 51-590, 1-27-89). As cited in; California EPA Dept of Pesticide Regulation Medical Toxicology Branch. Summary of Toxicology Data Didecyldimehylammoniumchloride revised 2/14/1996. http://www.cdpr.ca.gov/docs/toxsums/pdfs/1682.pdf

(8) Estimation conducted using KOWWIN Program (v1.66) as found in EPIWIN 3.05, Syracuse Research Corporation, ES EPA Version 2000, calculation by Toxicology and Regulatory Affairs, December 2003.

(9) Material Safety Data Sheet, BQAOH, Solutia MSDS No.: 0656523448 September 2, 1998

(10) MPBPWIN (v1.40) program as found in EPIWIN 3.05, Syracuse Research Corporation, ES EPA Version 2000

(11) MPBPWIN (v1.40), HENRY and Volatilization programs as found in EPIWIN 3.05, Syracuse Research Corporation, ES EPA Version 2000

(12) Mutagenicity Test on Didecyldimethylammoniumchloride (DDAC) in the CHO/HGPRT Forward Mutation Assay" (Young, R.R., Hazleton Laboratories America, Inc., Study No. 10141-0-435, 9-9-88). As cited in; California EPA Dept of Pesticide Regulation Medical Toxicology Branch. Summary of Toxicology Data Didecyldimehylammoniumchloride revised 2/14/1996. http://www.cdpr.ca.gov/docs/toxsums/pdfs/1682.pdf

(13) Two-Generation Reproduction Study in Sprague-Dawley (CD.) Rats with Didecyldimethylammoniumchloride Administered in the Diet", (T.L. Neeper-Bradley, Bushy Run Research Center, Export, PA., Report # 52-648, 2/1/91). As cited in; California EPA Dept of Pesticide Regulation Medical Toxicology Branch. Summary of Toxicology Data Didecyldimehylammoniumchloride revised 2/14/1996. http://www.cdpr.ca.gov/docs/toxsums/pdfs/1682.pdf

(14) Younger Laboratories Inc, Final Report: Acute Toxicity Testing of BQAOH, project YO-81-063, 11-6-1981; sponsored by Monsanto Co.